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Three-dimensional structure of phosphorus-containing heterocycles - II. Dipole moments and Kerr constants of some 2-thiono-1,3,2-dioxaphosphorinanes

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Abstract

The three-dimensional structure of a number of 2-thiono-1,3,2-dioxaphosphorinanes was studied by means of dipole moments, the Kerr effect, and theoretical conformational analysis with P^{31} NMR data. 2,4-Dimethyl- and 2-chloro-2-thiono-1,3,2-dioxaphosphorinanes have the chair conformation with an equatorial thionophosphoryl group; the 2-methyl derivative exist as an equilibrium mixture of the axial and equatorial conformers with predominance of the former. The participation of the boat form in the conformational equilibrium was established for 2-chloro-4-methyl derivative. © 1974 Consultants Bureau.

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